

Charge pairing and superconductivity in high- T_c cuprate superconductors

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We propose a model for high- T_c superconductors that includes both the spin fluctuations of the Cu^{++} magnetic ions and of the spins of O^{--} doped holes (spinons). The charge of the dopants (holons) is associated to quantum skyrmion excitations of the Cu^{++} spin background. The quantum skyrmion effective interaction potential is evaluated as a function of doping and temperature, indicating that Cooper pair formation is determined by the competition between these two types of spin fluctuations. The superconducting transition occurs when the effective potential allows for skyrmion bound states. Our theoretical predictions for the superconducting phase diagram of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ and $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ are in good agreement with experiment.

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Introduction. High-temperature underdoped cuprates exhibit a wide variety of interesting physical phenomena, like Néel and metal-insulator transitions, non-Fermi liquid behavior, pseudogap, etc., and have inspired a large amount of theoretical and experimental work for about fifteen years. In spite of that, even the nature of the ground state and of its elementary excitations, have not yet been fully determined and many different pictures are available [1].

Another fundamental point yet to be understood is the mechanism of charge pairing. It is by now well established that antiferromagnetic spin correlations play an important role in the dynamics of the system, even after the destruction of the Néel state. Indeed, different spin-fluctuation models have been successfully used to explain the observed spectral weight in ARPES data of high- T_c materials [2], as well as other anomalies [3]. Moreover, the idea of spin-fluctuation induced charge pairing and superconductivity has been used recurrently [4].

In this work we propose a theory for high- T_c cuprates that takes into account the spin fluctuations of the Cu^{++} magnetic ions and of the O^{--} doped holes as independent degrees of freedom. The charge of the dopants (holons) is associated to skyrmion quantum spin excitations of the Cu^{++} background, which in the Néel phase are finite energy defects closely related to their classic counterparts whereas in the quantum disordered phase are nontrivial zero energy purely quantum mechanical excitations. The spin of the doped holes (spinons), on the other hand, is represented by chargeless, massless Dirac fermion fields [5]. We calculate the effective interaction potential between these quantum skyrmion topological excitations in order to study charge pairing. It becomes clear that Cooper pairing is controlled by the competition between the spin fluctuations of Cu^{++} magnetic ions and those of the O^{--} doped holes. Our predictions for the T_{SC} line are in good agreement with experiment for both $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ and $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$.

The model. Our starting point will be the generalized spin-fermion model described by the Hamiltonian

$$\mathcal{H} = -t_p \sum_{\langle i,j \rangle, \alpha} (c_{i,\alpha}^\dagger c_{j,\alpha} + h.c.) + U_p \sum_{i,\alpha} n_{i,\alpha} n_{i,\alpha} + J_K \sum_{i,\alpha,\beta} \vec{S}_i \cdot c_{i,\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{i,\beta} + J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j, \quad (1)$$

which arises from the strong coupling limit of the three band Hubbard Model (3BHM) [6]. In the above expression, \vec{S}_i represent the localized spins of Copper ions, which interact through the superexchange J , $c_{i,\alpha}^\dagger$, $\alpha = 1..N = 2$, is the hole creation operator, t_p is the hopping term for holes, J_K is a Kondo like coupling between the spins of Cu^{++} ions and the spins of O^{--} holes, and we have retained the usually ignored onsite Coulomb repulsion between O^{--} holes, $U_p \neq 0$ with $n_{i,\alpha} = c_{i,\alpha}^\dagger c_{i,\alpha}$. The reason is that realistic estimates from the 3BHM suggest that $U_p/t_p \sim 10$ [7], being rather large, and thus we can perform a t_p/U_p expansion. Second order perturbation theory in t_p/U_p will give rise to a superexchange $J_p = 2t_p^2/U_p$ between oxygen spins and we end up with a $t - J$ model for the holes.

The mean field (large N) solutions of the $t - J$ model are well known and it has been established that a π -flux phase has minimum energy, at least at the saddle-point level ($N \rightarrow \infty$) [5]. We can write the electron in terms of a charged spinless boson μ_i (holon) and a chargeless spin-1/2 fermion $f_{i,\alpha}$ (spinon), and, as usual, we decouple the four particle interactions by introducing the d -wave auxiliary fields $\chi_{ij} = \langle f_{i,\alpha}^\dagger f_{j,\alpha} \rangle$ and $\Delta_{ij} = \langle f_{i,\uparrow} f_{j,\downarrow} - f_{i,\downarrow} f_{j,\uparrow} \rangle$, which are nonzero for $T < T^*$, where T^* is the pseudogap temperature. If we then neglect charge fluctuations, $\langle \mu_i \mu_j^\dagger \rangle \simeq |\mu_i|^2 = \text{const.}$, we find that the lowest lying excitations of the π -flux phase are massless, chargeless, spin carrying Dirac Fermi fields [5] whose dynamics is described by the Lagrangian

$\mathcal{L} = \sum_{\alpha,\lambda} i\bar{\psi}_{\alpha,\lambda} \left(\gamma_0 \partial_\tau - v_F \vec{\gamma} \cdot \vec{\nabla} \right) \psi_{\alpha,\lambda}$, where $\lambda = 1, 2$ label the two Fermi points at $(\pi/2, \pm\pi/2)$, $\partial_\mu = (\partial_\tau, \vec{\nabla})$, $\gamma_\mu = (\gamma_0, \vec{\gamma}) = (i\sigma_z, \sigma_x, \sigma_y)$, $v_F = 2a\chi$ is the dopant Fermi velocity (with a being the lattice spacing and χ the constant amplitude of $|\chi_{ij}|$) and $\psi_{\alpha,\lambda} = \begin{pmatrix} f_{\alpha,\lambda}^e \\ f_{\alpha,\lambda}^o \end{pmatrix}$, for (o)dd and (e)ven lattice sites. The long wavelength fluctuations of the localized Cu^{++} spins, on the other hand, are described by the CP^{N-1} Lagrangian $\mathcal{L}_{\text{CP}^{N-1}} = (1/2g_0) |(\partial_\mu - i\mathcal{A}_\mu)z_i|^2$, where $\vec{S} = z_i^\dagger \vec{\sigma}_{ij} z_j$, with z_i^\dagger, z_i , $i = 1..N = 2$, being Schwinger boson fields such that $z_i^\dagger z_i = 1$, $\mathcal{A}_\mu = -i\bar{z}_i \partial_\mu z_i$, and g_0 is a bare coupling constant. It is now convenient to perform the local canonical transformation $\psi \rightarrow U\psi$, where $U = \exp \left[q \begin{pmatrix} z_1 & -\bar{z}_2 \\ z_2 & \bar{z}_1 \end{pmatrix} \right] \in \text{SU}(2)$, and q is arbitrary. Now the Kondo coupling term in (1) reduces to a chemical potential term, since $U^\dagger \vec{S} \cdot \vec{\sigma} U = \sigma_z$. Also, since $U^\dagger \partial_\mu U = iq\sigma_z \mathcal{A}_\mu + \text{negligible nondiagonal terms}$, we end up with the effective theory

$$\mathcal{Z} = \int \mathcal{D}\bar{z} \mathcal{D}z \mathcal{D}\bar{\psi} \mathcal{D}\psi \mathcal{D}\mathcal{A}_\mu \delta[\bar{z}z - 1] e^{-S}, \quad (2)$$

where

$$S = \int_0^{\beta\hbar} d\tau \int d^2\mathbf{x} \left\{ \sum_{i=1..N} \frac{1}{2g_0} |(\partial_\mu - i\mathcal{A}_\mu)z_i|^2 + \sum_{\alpha=1..N, \lambda=1,2} \bar{\psi}_{\alpha,\lambda} \gamma_\mu (i\partial^\mu - q\sigma_z \mathcal{A}^\mu) \psi_{\alpha,\lambda} \right\}. \quad (3)$$

Holons as quantum skyrmions. In previous works [8], we have proposed a model for doping quantum Heisenberg antiferromagnets, that successfully described the magnetization curves and the AF part of the phase diagrams of both LSCO and YBCO. One of the important consequences of that model was the observation that each hole added to the CuO_2 planes creates a skyrmion topological defect on the Cu^{++} spin background, in agreement with earlier proposals [9]. The dopant charge, in particular, was found to be attached to the skyrmion charge and consequently its dynamics becomes totally determined by the quantum skyrmion correlation functions. Despite the fact that the model proposed in [8] is restricted to the antiferromagnetic part of the phase diagram, we shall nevertheless pursue the picture in which skyrmions are in general the charge carriers of the doped holes. This will allow us to treat the bosonic variable μ_i introduced above as a quantum skyrmion operator. In particular, we shall exploit this idea in the quantum disordered phase, $\delta \geq \delta_{AF}$, where the skyrmions are purely quantum mechanical and have zero energy.

The full treatment of the quantum skyrmions of the theory described by (3) has been carried out in [10]. In

the renormalized classical regime, $g_0 < g_c$ ($g_c = 8\pi/\Lambda$), we have

$$\langle \mu(x) \mu^\dagger(y) \rangle = \frac{e^{-2\pi\rho_s|x-y|}}{|x-y|^{q^2/2}}, \quad (4)$$

where $\rho_s = 1/g_0 - 1/g_c$. Conversely, for the theory studied in [8] the corresponding correlator was found to be

$$\langle \mu(x) \mu^\dagger(y) \rangle = \frac{e^{-2\pi\rho_s(\delta)|x-y|}}{|x-y|^{\alpha(\delta)}}, \quad (5)$$

where the expressions for $\rho_s(\delta)$ and $\alpha(\delta)$ have been carefully determined in [8]. In particular, $\alpha(\delta) = \left[\frac{64}{\pi^2+16} + \frac{\alpha_{EM}}{4\pi^2} \right] (n\delta)^2$ with $n = 1$ for YBCO and $n = 4$ for LSCO, the factor of four being a consequence of the existence of four branches in the Fermi surface for this compound, as discussed in [8]. α_{EM} is the electromagnetic fine structure constant and we see that the contribution from the electromagnetic coupling is negligible. The $\rho_s(\delta)$ function is given by $\rho_s(\delta) = \rho_s(0)[1 - A\delta^2]$, for YBCO and $\rho_s(\delta) = \rho_s(0)[1 - B\delta - C\delta^2]^{1/2}$, for LSCO, and again the different behavior being ascribed to the form of the Fermi surface in each case [8]. The constants A, B and C have been evaluated from first principles in [8]. In order to obtain the δ -dependence of the spin stiffness ρ_s and of the spinon coupling q in our model (3), we now match the two correlation functions in (4) and (5) (ordered phase), obtaining $\rho_s = \rho_s(\delta)$ and $q = \left[\frac{128}{\pi^2+16} \right]^{1/2} (n\delta)$. The sublattice magnetization in the ordered phase is given by $M(\delta) = \sqrt{\rho(\delta)}$, and consequently δ_{AF} can be obtained from $\rho(\delta_{AF}) = 0$, both in good agreement with experiment, see [8]. For $\delta > \delta_{AF}$, on the other hand, where $\rho_s = 0$, we shall assume that the expression for $q(\delta)$ still holds. This is quite reasonable since q was introduced by a local canonical transformation, and at least locally there is short range AF order.

Cooper pair formation. Let us now investigate the conditions for Cooper pairing. We shall first introduce in the partition function (2) the skyrmion current, $\mathcal{J}^\mu = \frac{1}{2\pi} \epsilon^{\mu\alpha\beta} \partial_\alpha \mathcal{A}_\beta$, through the identity

$$1 = \int \mathcal{D}\mathcal{J}_\mu \delta[\mathcal{J}_\mu - \frac{1}{2\pi} \epsilon^{\mu\alpha\beta} \partial_\alpha \mathcal{A}_\beta]. \quad (6)$$

Integrating over z_i^\dagger, z_i and $\bar{\psi}_a, \psi_a$, we obtain, at leading order, the effective Lagrangian

$$\mathcal{L}_{eff}[\mathcal{A}_\mu] = \frac{N}{2} \mathcal{A}_\mu(\mathbf{x}, \tau) \Pi^{\mu\nu}(\mathbf{x} - \mathbf{y}, \tau - \tau') \mathcal{A}_\nu(\mathbf{y}, \tau'), \quad (7)$$

where $\Pi^{\mu\nu}(\mathbf{x} - \mathbf{y}, \tau - \tau')$ has Fourier transform given by $\Pi^{\mu\nu}(\mathbf{p}, i\epsilon_m) = \Pi_B^{\mu\nu}(\mathbf{p}, i\epsilon_m) + \Pi_F^{\mu\nu}(\mathbf{p}, i\epsilon_m)$, which are respectively the contributions to the finite temperature vacuum polarization coming from the complex scalar fields z_i (Schwinger bosons) and fermions $\psi_{\alpha,\lambda}$ (spinons).

In order to obtain the effective current-current interaction between skyrmions, we use an exponential representation for the δ -function in (6) and integrate over \mathcal{A}_μ and the corresponding Lagrange multiplier field. The result is

$$\mathcal{Z} = \int \mathcal{D}\mathcal{J}_\mu e^{\{-2\pi^2 \int d^3x \int d^3y \mathcal{J}_\mu(x) \Sigma^{\mu\nu}(x-y) \mathcal{J}_\nu(y)\}}, \quad (8)$$

where $\Sigma^{\mu\nu}(p) = \Pi^{\mu\nu}(p)/p^2$, $x = (\tau, \mathbf{x})$ and $p = (i\epsilon_m, \mathbf{p})$. The real time effective interaction energy between static skyrmions ($\epsilon_m = 0$) is then

$$\mathcal{H}_I = 2\pi^2 \int d^2\mathbf{x} \int d^2\mathbf{y} \rho(\mathbf{x}) \Sigma^{00}(\mathbf{x} - \mathbf{y}; 0) \rho(\mathbf{y}), \quad (9)$$

where $\rho(\mathbf{x}) = \mathcal{J}_0(\mathbf{x})$ is the dopant charge density and $\Sigma^{00}(\mathbf{x} - \mathbf{y}; 0)$ has Fourier transform given by $\Sigma^{00}(\mathbf{p}) = \Pi_B(\mathbf{p}) + \Pi_F(\mathbf{p})$ with

$$\begin{aligned} \Pi_B(\mathbf{p}) = & -\frac{\Delta}{2\pi} + \frac{1}{2\pi} \int_0^1 dx \sqrt{|\mathbf{p}|^2 x(1-x) + m^2} \\ & \times \coth\left(\frac{\sqrt{|\mathbf{p}|^2 x(1-x) + m^2}}{2k_B T}\right), \end{aligned} \quad (10)$$

and

$$\Pi_F(\mathbf{p}) = \frac{q^2}{\pi} \int_0^1 dx \sqrt{|\mathbf{p}|^2 x(1-x)} \tanh\left(\frac{\sqrt{|\mathbf{p}|^2 x(1-x)}}{2k_B T}\right). \quad (11)$$

In the above expressions, m is the inverse correlation length of the quantum disordered phase of the CP^{N-1} model, where $\Delta = 8\pi(1/g_c - 1/g_0)$ and $\rho_s = 0$. At order N , it is given exactly by $m(T) = \Delta + 2k_B T e^{-\Delta/k_B T}$ [11].

For two charges at positions \mathbf{x}_1 and \mathbf{x}_2 , we have $\rho(\mathbf{x}) = \delta^{(2)}(\mathbf{x} - \mathbf{x}_1) + \delta^{(2)}(\mathbf{x} - \mathbf{x}_2)$. After discarding self-interactions, we obtain ($\mathbf{r} = \mathbf{x}_1 - \mathbf{x}_2$)

$$V(\mathbf{r}) = \int d^2\mathbf{p} \Sigma^{00}(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{r}} + V_l(\mathbf{r}), \quad (12)$$

where we have also introduced the centrifugal barrier potential between the two charges that form the Cooper pair, $V_l(\mathbf{r}) = l(l+1)\hbar^2/2M^*\mathbf{r}^2$, with l specifying the relative orbital angular momentum of the pair and M^* the effective mass of the charges.

Zero temperature limit. It is well known that in high- T_c cuprates, Cooper pairs form at relatively short distances. In this limit, large $|\mathbf{p}|$, we have, at $T = 0$

$$V(\mathbf{r}) \rightarrow \int d^2\mathbf{p} \left[\frac{1}{8|\mathbf{p}|} - \frac{2q^2}{8|\mathbf{p}|} \right] e^{i\mathbf{p}\cdot\mathbf{r}} + V_l(\mathbf{r}). \quad (13)$$

The above expression clearly shows a competition between the spin fluctuations of the Cu^{++} spins (first term) and of the O^{--} doped spins (second term). For small

enough doping, $q^2 < 1/2$, the potential is always repulsive and there is no charge pairing. For $q^2 > 1/2$, on the other hand, the potential has a minimum and charge (skyrmion) pairing occurs. We conclude that the critical doping for the onset of superconductivity is determined by the condition $q^2(\delta_{SC}) = 1/2$. We observe that without the Cu^{++} background, the interaction potential (13) would always have bound states for any $q \neq 0$, at zero temperature, and $\delta_{SC} = 0$. This is what happens in the mean field phase diagram of Kotliar and Liu [12]. We see that the effect of the Cu^{++} background is to shift the value of δ_{SC} to its correct position in the phase diagram.

Determination of δ_{SC} . From the expression of q in terms of δ ($q = \sqrt{2\alpha(\delta)}$), we see that δ_{SC} is only determined by the shape of the Fermi surface of the compound. In particular, we see that $\delta_{SC}^{YBCO} = 4\delta_{SC}^{LSCO}$, a result that is verified by experiments, if we take in account the relation between δ and the stoichiometric doping parameter x , namely $\delta = x$ for LSCO and $\delta = x - 0.20$ for YBCO. Another prediction of our model is that compounds with similar Fermi surfaces should have the same superconducting critical doping δ_{SC} . We get $\delta_{SC}^{YBCO} = 0.318$ and $\delta_{SC}^{LSCO} = 0.079$, which have a fairly good agreement with experiment.

Disorder. Disorder may be modelled in the ordered Néel phase of a doped antiferromagnet by considering a continuous random distribution of spin stiffnesses [13]. The effect of introducing a Gaussian $\times |\rho - \rho_s|^{\nu-1}$ distribution, with exponentially suppressed magnetic dilution, in the original model [8], is a correction for $\alpha(\delta)$, namely $\alpha(\delta) \rightarrow \alpha'(\delta) = \alpha(\delta) + \nu$ [13]. Choosing $\nu = \frac{1}{8}$ for both compounds, we get $\delta_{SC} = \frac{1}{n} \sqrt{\frac{\pi^2 + 16}{512}}$, or equivalently $x_{SC}^{YBCO} = 0.425$ and $x_{SC}^{LSCO} = 0.056$, in good agreement with experiment.

Finite temperature. For Π_B we shall expand in $k_B T/m$, since it is clear that $m(T) > k_B T, \forall T$. Π_B will then be simply given by its zero temperature limit, where $m = \Delta$. For Π_F , on the other hand, such a low T expansion is not necessarily valid even for $|\mathbf{p}| \gg k_B T$. We will then have to split the integral over the Feynman parameter x in (11) into three parts. For $0 \leq x \leq x_c$ and $1 - x_c \leq x \leq 1$, $x_c = (k_B T/|\mathbf{p}|)^2$, we will use a high T expansion, while for $x_c \leq x \leq 1 - x_c$ we use the low T expression. We obtain

$$\Sigma^{00}(\mathbf{p}) = \frac{(1 - 2q^2)}{8|\mathbf{p}|} - \frac{m}{\pi|\mathbf{p}|^2} + \frac{m^2}{2|\mathbf{p}|^3} + \frac{16q^2 T^3 - 4m^3}{3\pi|\mathbf{p}|^4}. \quad (14)$$

Inserting this in (12), we get $V(\mathbf{r})$, and from the threshold conditions for the formation of bound states, namely $V'(\mathbf{r}_0) = 0$ and $V''(\mathbf{r}_0) = 0$, we obtain the relation

$$(k_B T_{SC})^3 = -\frac{\pi(1 - 2q^2)\alpha^3}{512q^2} + \frac{m\alpha^2}{32q^2} - \frac{3\pi m^2 \alpha}{128q^2} + \frac{m^3}{4q^2}$$

$$- \frac{3\pi^2 l(l+1)\alpha^4}{q^2 M^* v_F^2}, \quad (15)$$

where $\alpha = \hbar v_F / r_0$, $m = \Delta$, and r_0 is the minimum of the potential (it also measures the size of the Cooper pair).

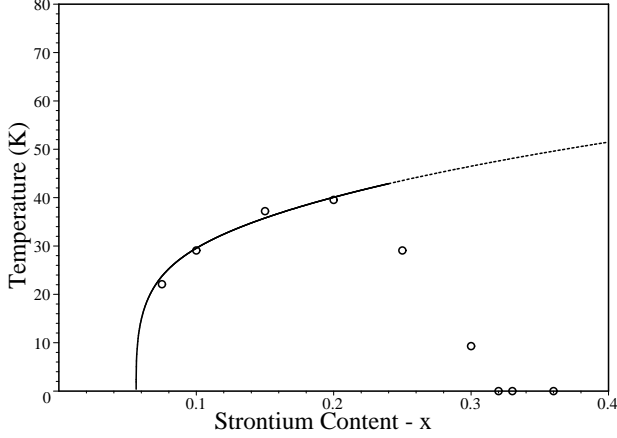


FIG. 1. Plot of curve (15) for $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$. Experimental data from [14].

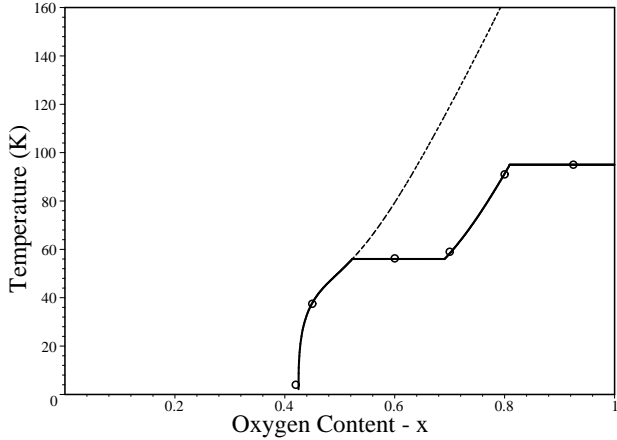


FIG. 2. Plot of curve (15) for $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$. Experimental data from [15].

Comparison with experiment. In order to make contact with experimental data we need the doping dependence of Δ . For YBCO, we use $\Delta(\delta) = \Delta_0[(\delta/\delta_{AF})^2 - 1]$, in agreement with the results of [8], with $\Delta_0 = 8.8$ meV. For LSCO, we shall use an expression that fits the experimental data of [14], namely $\Delta(\delta) = \Delta_0[(\delta/\delta_{AF})^2 - 1]^{1/2}$, with $\Delta_0 = 1.0$ meV. For the $T = 0$ AF quantum critical point δ_{AF} , we know from experiments that $\delta_{AF} = 0.22$ for YBCO and $\delta_{AF} = 0.02$ for LSCO. Inserting in (15) the values of δ_{SC} at $T = 0$, obtained previously, we get a relation that fixes $M^* v_F^2$ with respect to r_0 . In figs. 1 and 2 we plot the curve (15) for LSCO and YBCO, respectively, with $r_0 = 38$ Å, $\hbar v_F = 0.18$ eV Å for LSCO and $\hbar v_F = 1.08$ eV Å for YBCO, and $l = 2$ (d -wave pairing). In the first plot (LSCO), the dashed part is in the region where $T > T^*$ and we should move to a

new saddle-point. In the second plot (YBCO) we have shifted the curve (dashed part) to the right in the regions $\delta = [0.52, 0.7]$ and $\delta = [0.8, 1]$ in order to comply with the effects of the out-of-plane O-Cu-O chains, which produce the observed 60 K and 90 K plateaus, where the extra holes do not enter in the CuO_2 planes. Furthermore, for YBCO, T^* is higher than T_{max} ($\delta = 1$) and therefore imposes no restrictions to our results.

Final remarks. We would like to remark that our theory (3) also gives a simple interpretation for the pseudogap phenomena. Indeed, for $T_{SC} < T < T^*$ spinons are paired into d -wave singlets but holons (skyrmions) repel each other and there is no superconducting state. Only for $T < T_{SC}$ we do have Cooper pair formation and superconductivity.

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